LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-GF-02-067-A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029035.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	378	384	395	rBB	203113	280706	64.70%	8.952%
2	6.869	654	660	670	rBV	179392	278386	64.17%	8.878%
3	7.669	791	796	802	rBB	49460	71086	16.39%	2.267%
4	8.845	989	996	1004	rBV	111696	178482	41.14%	5.692%
5	10.463	1265	1271	1277	rBV	57516	90005	20.75%	2.870%
6	12.951	1688	1694	1702	rVB	242581	336043	77.46%	10.717%
7	14.057	1878	1882	1888	rBV	3282	4828	1.11%	0.154%
8	14.210	1899	1908	1919	rBV4	6203	17644	4.07%	0.563%
9	14.339	1924	1930	1936	rVB2	74426	105714	24.37%	3.371%
10	15.833	2179	2184	2192	rBV	175995	238840	55.05%	7.617%
11	17.086	2388	2397	2401	rBV	85248	113532	26.17%	3.621%
12	17.127	2401	2404	2412	rVB	17164	21617	4.98%	0.689%
13	17.215	2414	2419	2425	rBV	6053	8466	1.95%	0.270%
14	17.980	2541	2549	2560	rBV2	36293	56046	12.92%	1.787%
15	18.151	2572	2578	2582	rBV3	5261	9054	2.09%	0.289%
16	19.139	2739	2746	2753	rBV	52962	69895	16.11%	2.229%
17	19.262	2762	2767	2771	rBV3	20333	25647	5.91%	0.818%
18	19.474	2799	2803	2804	rBV	8373	9999	2.30%	0.319%
19	19.503	2804	2808	2812	rVB	43945	54860	12.65%	1.750%
20	19.709	2838	2843	2848	rVB	370498	433826	100.00%	13.836%
21	19.827	2860	2863	2871	rBV6	2626	5236	1.21%	0.167%
22	19.998	2884	2892	2898	rBV4	9041	20128	4.64%	0.642%
23	20.098	2905	2909	2913	rBV	6717	9248	2.13%	0.295%
24	20.156	2915	2919	2922	rVB2	4126	6590	1.52%	0.210%
25	20.345	2946	2951	2954	rBV5	5589	7322	1.69%	0.234%
26	20.939	3050	3052	3054	rBV	5907	6656	1.53%	0.212%
27	20.974	3054	3058	3067	rVB4	52891	77140	17.78%	2.460%
28	21.256	3100	3106	3110	rBV2	124913	199235	45.93%	6.354%
29	21.292	3110	3112	3117	rVB	31860	36527	8.42%	1.165%
30	21.409	3129	3132	3136	rBV4	8997	13022	3.00%	0.415%
31	21.844	3204	3206	3211	rVB6	15340	17615	4.06%	0.562%
32	22.774	3361	3364	3375	rVB	33650	102417	23.61%	3.266%
33	23.233	3438	3442	3446	rVB	19052	29029	6.69%	0.926%
34	23.321	3454	3457	3467	rVB	29709	54926	12.66%	1.752%
35	23.415	3468	3473	3479	rBV2	80740	145766	33.60%	4.649%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

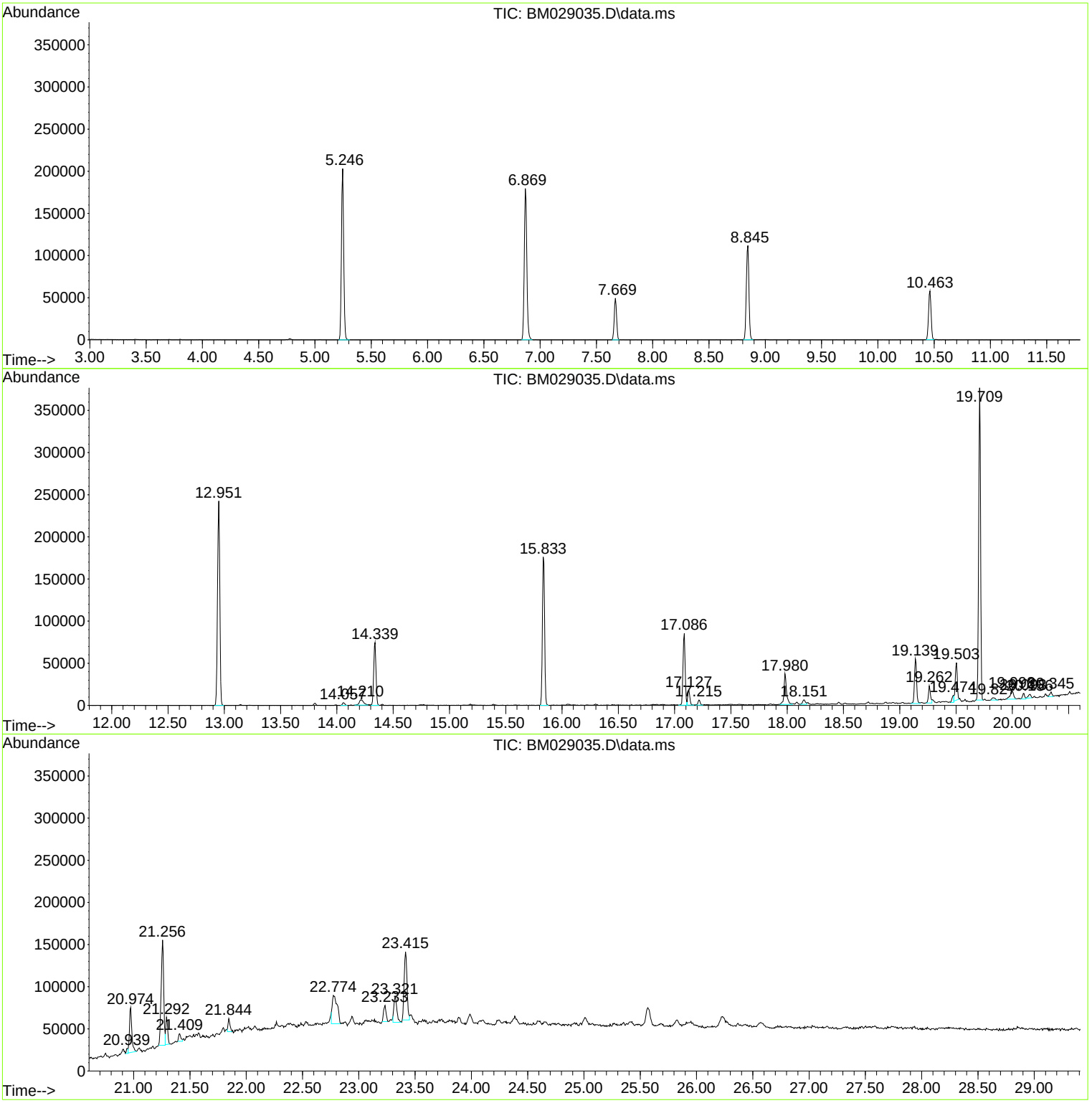
Sum of corrected areas: 3135533

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
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Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-A

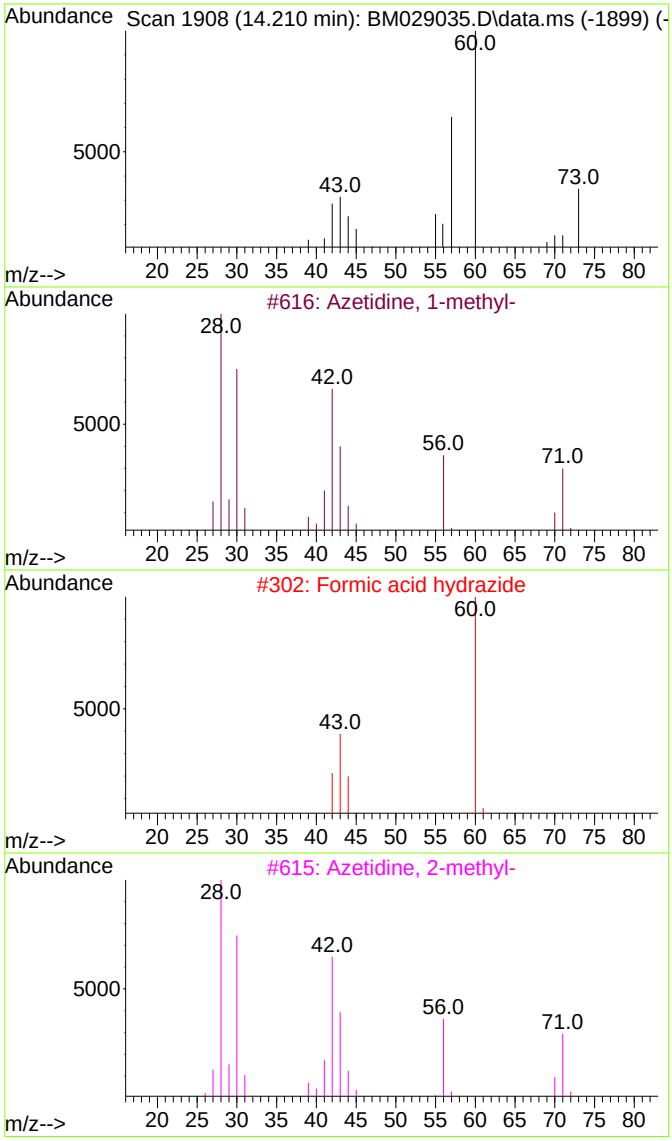
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

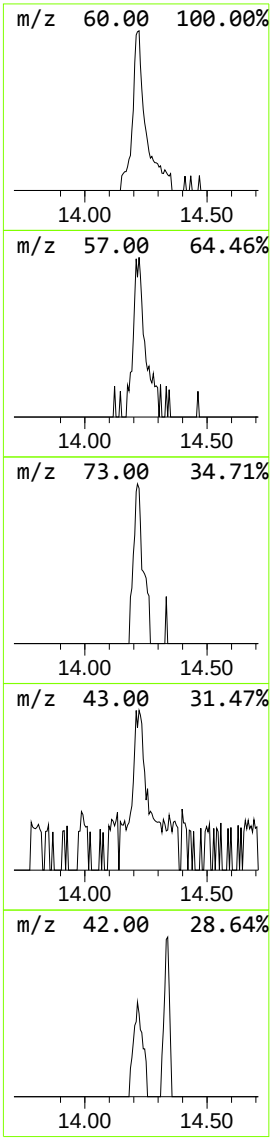
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown14.210 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	3.34 ng	17644	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	9
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	9
4	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
5	Butanoic acid	88	C4H8O2	000107-92-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

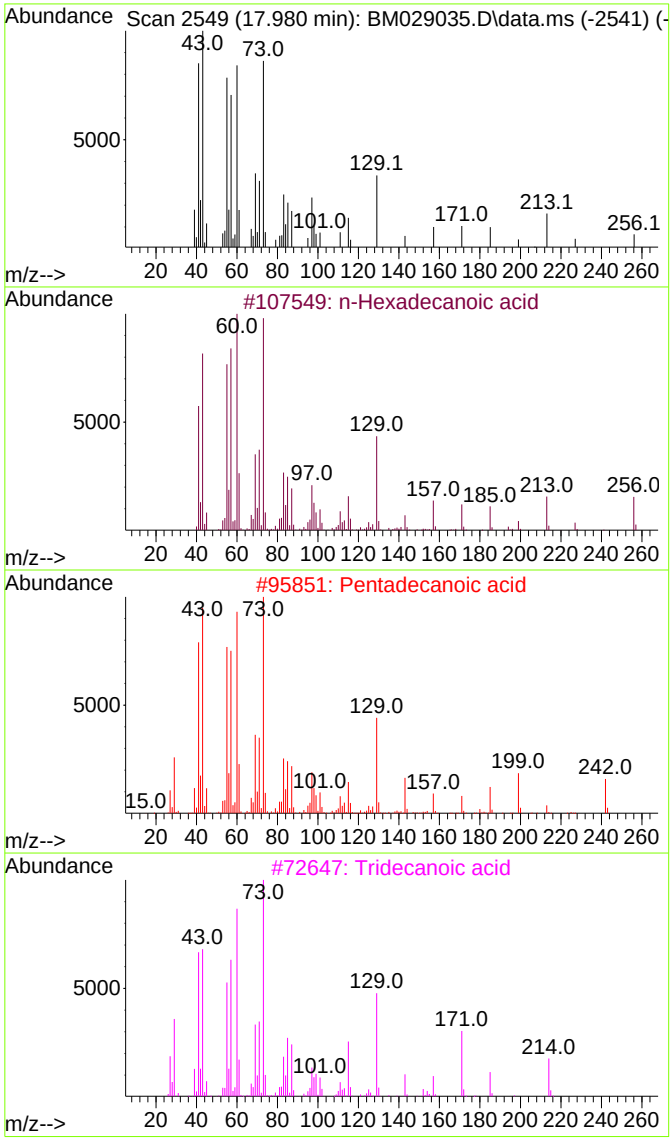
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

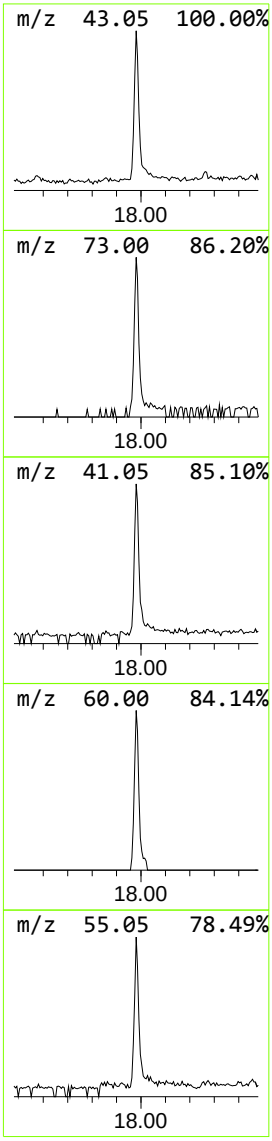
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	9.87 ng	56046	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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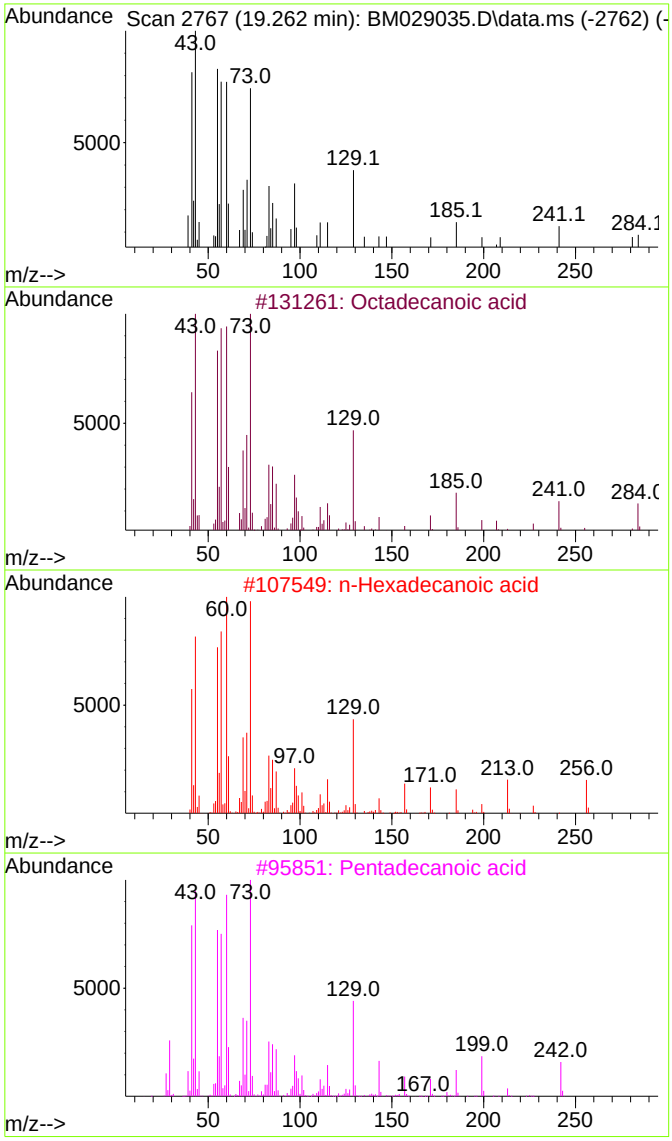
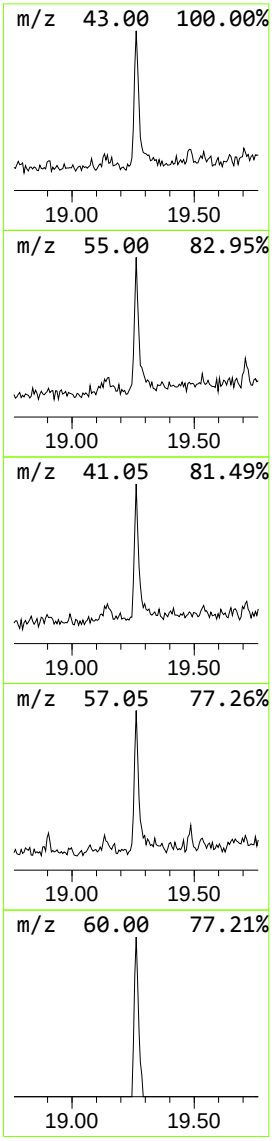
Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.262	2.57 ng	25647	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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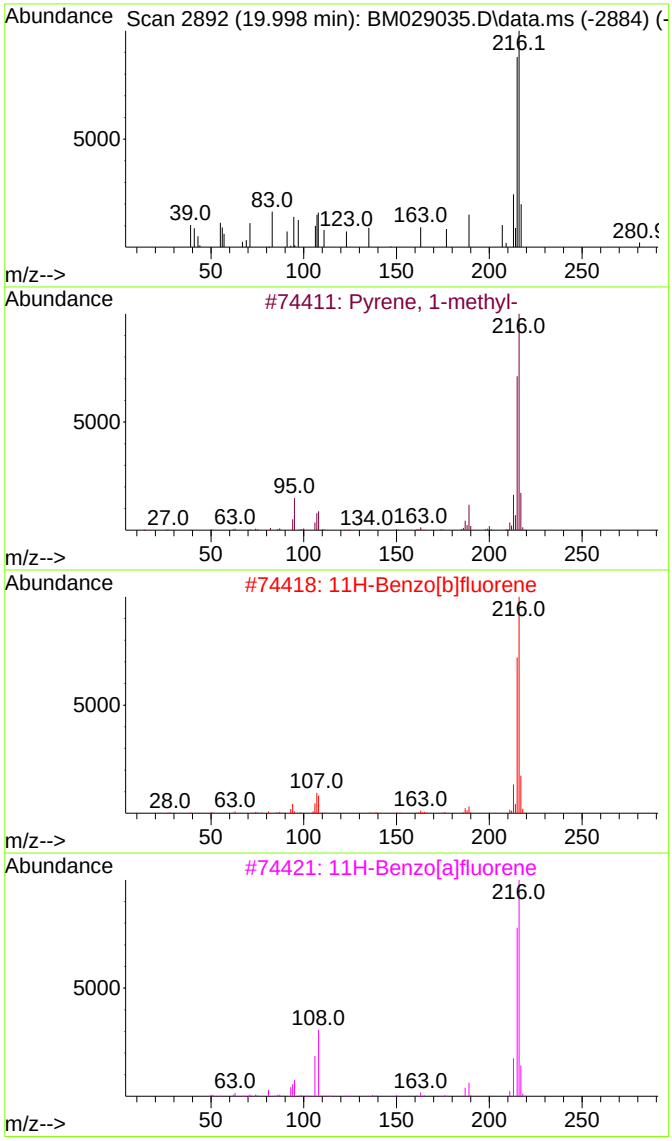
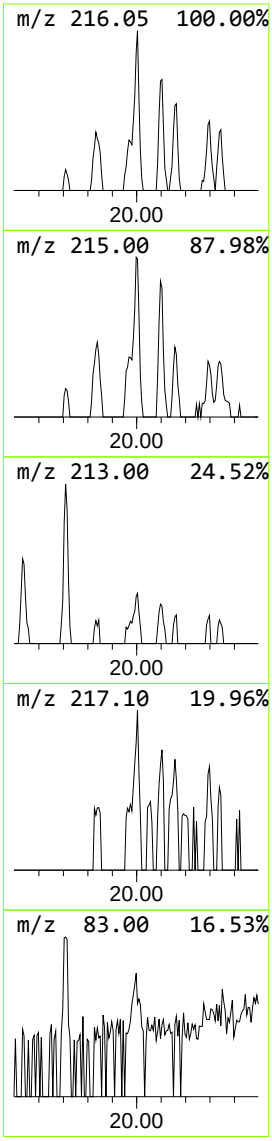
Peak Number 4 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.998	2.02 ng	20128	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	80
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64





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Operator : CG/JU
Sample : M1589-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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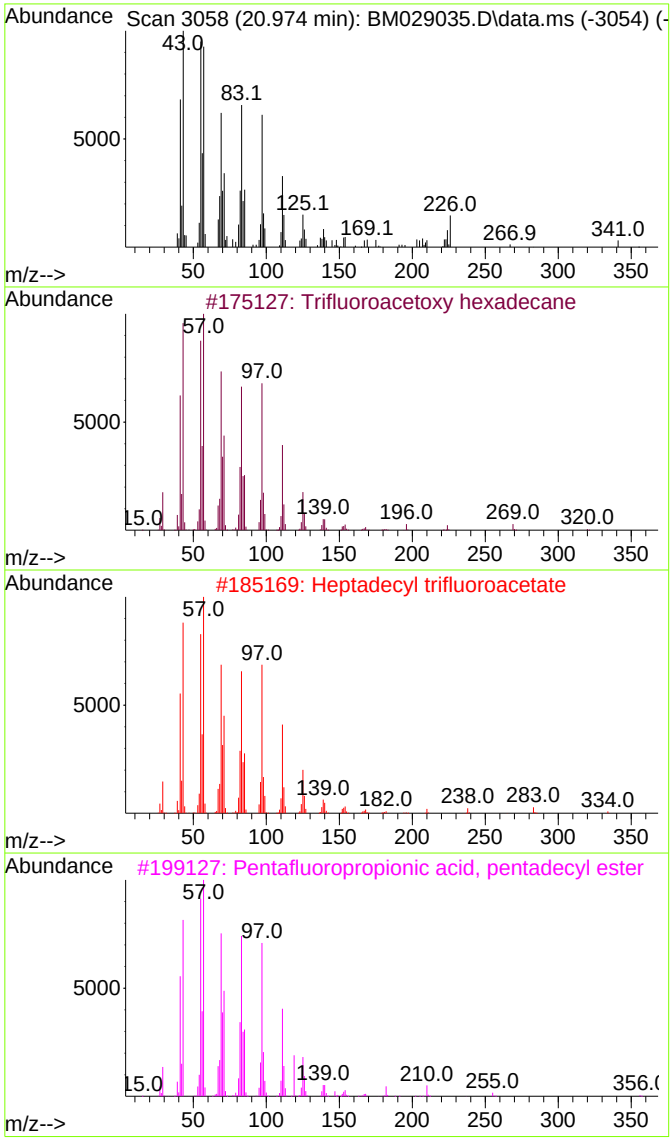
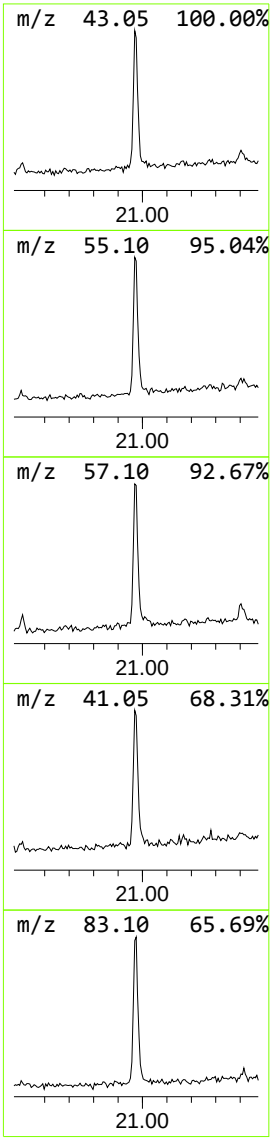
Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	7.74 ng	77140	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
5	Z-8-Hexadecene	224	C16H32	1000130-87-5	91





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Sample : M1589-01
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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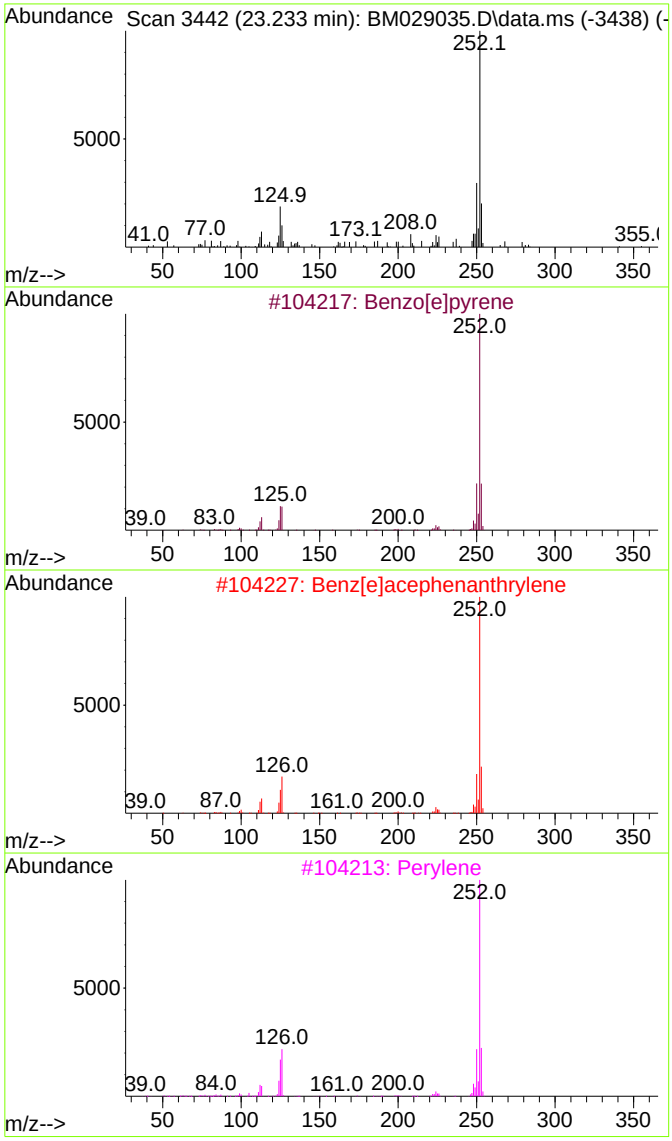
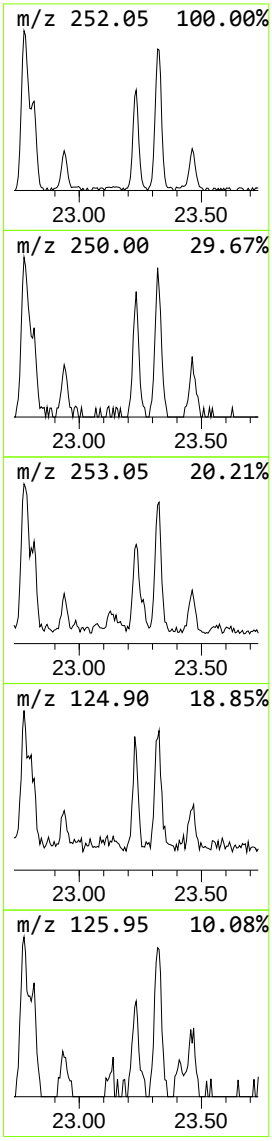
Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.233	3.98 ng	29029	Perylene-d12	23.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	89
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	70
3	Perylene	252	C20H12	000198-55-0	70
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	70
5	Benzo[a]pyrene	252	C20H12	000050-32-8	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029035.D
Acq On : 09 Mar 2021 00:58
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Instrument : BNA_M
ClientSampleId : FK-GF-02-067-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown14.210	14.210	3.3	ng	17644	3	14.339	105714	20.0
n-Hexadecanoic ...	17.980	9.9	ng	56046	4	17.086	113532	20.0
Octadecanoic acid	19.262	2.6	ng	25647	5	21.256	199235	20.0
Pyrene, 1-methyl-	19.998	2.0	ng	20128	5	21.256	199235	20.0
Trifluoroacetox...	20.974	7.7	ng	77140	5	21.256	199235	20.0
Benzo[e]pyrene	23.233	4.0	ng	29029	6	23.415	145766	20.0